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A history of Runge–Kutta methods

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Abstract

This paper constitutes a centenary survey of Runge–Kutta methods. It reviews some of the early contributions due to Runge, Heun, Kutta and Nyström and leads on to the theory of order of accuracy of Runge–Kutta methods, and includes a discussion of implicit methods, stability analysis and methods of error estimation and dense output.

1. Introduction

One hundred years ago, C. Runge was completing his famous paper. This work, published in 1895, extended the approximation method of Euler to a more elaborate scheme which was capable of greater accuracy. The idea of Euler was to propagate the solution of an initial value problem forward by a sequence of small time-steps. In each step, the rate of change of the solution is treated as constant and is found from the formula for the derivative evaluated at the beginning of the step.

For the equation $y'(x) = f(x, y(x))$, with given initial value $y(x_0) = y_0$, the first step is from the initial x_0 to a slightly larger value x_1, say. The approximate solution at this point is taken to be $y_1 = y_0 + (x_1 - x_0) f(x_0, y_0)$. In general for a sequence of time values $x_0, x_1, x_2, \ldots$, the corresponding solution approximations $y_0, y_1, y_2, \ldots$, are given by

$$y_n = y_{n-1} + (x_n - x_{n-1}) f(x_{n-1}, y_{n-1}).$$

This approximation can be viewed as an extension to differential equations of the quadrature formula

$$\int_{x_{n-1}}^{x_n} \phi(x)\,\mathrm{d}x = (x_n - x_{n-1})\phi(x_{n-1}).$$

The idea of Runge was to base the approximate solution, not on this unsymmetrical and relatively inaccurate Riemann rule, but on such improved formulas as the midpoint and trapezoidal rules. The requirement of evaluating the derivative at the midpoint or endpoint of a step not yet completed, was

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achieved by first performing an Euler type of calculation to obtain a preliminary approximation to the solution at one of these points.

This characteristic feature of Runge–Kutta methods, of evaluating the function f a number of times in working the way through each step, was thus established. We will survey in Section 2 the early work of Runge, and his immediate successors Heun and Kutta, in laying the foundations for these methods and developing practical methods of increasing accuracy and efficiency. We will also discuss the important work of Nyström in 1925.

In Section 3 we will discuss the conditions for a Runge–Kutta method to have a given order of accuracy. Although we will concentrate on the conditions for a general autonomous system of equations, we will also compare this theory with that for a single first order equation.

In Section 4 we will discuss the derivation of methods of increasingly high order, in the context of known order barriers. The complication of the relationship between attainable order and numbers of stages for classical (explicit) methods is in sharp contrast to the simplicity of the corresponding questions for the more general implicit Runge–Kutta methods introduced in Section 5. Other motivations for implicit methods are their uses in the solution of stiff differential equation systems. We will discuss the use of these methods for this purpose with special reference to their implementation costs.

Section 6 is devoted to stability questions for Runge–Kutta methods. Historically, these questions range from step-size limitations due to what is now called mild stiffness to the identification of implicit Runge–Kutta methods which exhibit A-stability or the nonlinear generalization known as algebraic stability.

Because of the need to select an efficient stepsize sequence automatically, local error estimation is necessary. Methods for achieving this, especially through computations performed within the same steps, are discussed in Section 7. This requires additional stages as does the provision of dense output for interpolation purposes, also considered in this final section.

2. Runge–Kutta methods 1895–1925

Throughout this paper, we will write h for the stepsize $x_1 - x_0$. We will mainly confine our discussions just to the first step because it is typical. Runge's paper of 1895 [32] dealt with an initial value problem of the form

$$y'(x) = f\big(x, y(x)\big), \qquad y(x_0) = y_0. \tag{2.1}$$

He explored three main schemes. We express these in his terminology together with the modern tableau notation.

$$\Delta y = f\big(x_0 + \tfrac{1}{2}\Delta x, y_0 + \tfrac{1}{2} f(x_0 y_0)\Delta x\big)\Delta x,$$

$$\begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ \hline & 0 & 1 \end{array}$$

$$\Delta y = \frac{f(x_0 y_0) + f\left(x_0 + \Delta x, y_0 + f(x_0 y_0)\Delta x\right)}{2}\Delta x,$$

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$$\Delta' y = f(x_0 y_0),$$
$$\Delta'' y = f(x_0 + \Delta x, y_0 + \Delta x)\Delta' y,$$
$$\Delta''' y = f(x_0 + \Delta x, y_0 + \Delta x)\Delta'' y,$$
$$\Delta y = \frac{\Delta' y + \Delta''' y}{2},$$

$$\begin{array}{c|ccc} 0 & & & \\ 1 & 1 & & \\ 1 & 0 & 1 & \\ \hline & \frac{1}{2} & 0 & \frac{1}{2} \end{array}$$

The first of these three methods is the midpoint rule adapted to ordinary differential equations while the second and third methods are different versions of the trapezoidal rule. The last of these methods suggests iterative computation of the stage values. However, more natural today would be the method

$$\begin{array}{c|ccc} 0 & & & \\ 1 & 1 & & \\ 1 & \frac{1}{2} & \frac{1}{2} & \\ \hline & \frac{1}{2} & 0 & \frac{1}{2} \end{array}$$

since this hints at the implicit trapeziodal rule method.

In 1900, K. Heun took the order conditions as far as 4 and introduced amongst other methods the following of third order

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{3} & \frac{1}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

The paper by W. Kutta, which appeared in 1901, took the analysis of Runge–Kutta methods as far as order 5. He made a complete classification of order 4 methods and introduced the famous method

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

In the work on 5th order methods, his work was incomplete in two different respects. His analysis was for a first order differential equation, rather than a system of equations. This distinction becomes significant for the first time at this order. Specifically there are 17 order conditions for a system but only 16 for a single equation. Thus, in principle, it is possible to find methods which have order p ($p \geqslant 5$) for a single equation but only $p-1$ for a system. The other sense in which the work of Kutta

is incomplete is that his order 5 methods have slight errors in them. As corrected (in the case of the second, by Nyström), they are given by the following tableaux

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{5} & \frac{1}{5} & & & & & \\
\frac{2}{5} & 0 & \frac{2}{5} & & & & \\
1 & \frac{9}{4} & -5 & \frac{15}{4} & & & \\
\frac{3}{5} & -\frac{63}{100} & \frac{9}{5} & -\frac{13}{20} & \frac{2}{25} & & \\
\frac{4}{5} & -\frac{6}{25} & \frac{4}{5} & \frac{2}{15} & \frac{8}{75} & 0 & \\
\hline
 & \frac{17}{144} & 0 & \frac{25}{36} & \frac{1}{72} & -\frac{25}{72} & \frac{25}{48}
\end{array}
$$

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{3} & \frac{1}{3} & & & & & \\
\frac{2}{5} & \frac{4}{25} & \frac{6}{25} & & & & \\
1 & \frac{1}{4} & -3 & \frac{15}{4} & & & \\
\frac{2}{3} & \frac{2}{27} & \frac{10}{9} & -\frac{50}{81} & \frac{8}{81} & & \\
\frac{4}{5} & \frac{2}{25} & \frac{12}{25} & \frac{2}{15} & \frac{8}{75} & 0 & \\
\hline
 & \frac{23}{192} & 0 & \frac{125}{192} & 0 & -\frac{27}{64} & \frac{125}{192}
\end{array}
$$

The first phase in the history of Runge–Kutta methods ended in the work of E.J. Nyström. He took the analysis of fifth order methods to its completion but, more importantly, he extended the use of Runge–Kutta methods to second order differential equation systems. These systems arise in dynamical problems and can often be solved more efficiently when posed in their original form rather than as converted to an equivalent first order system. Consider the special second order system

$$y''(x) = f(y(x)), \qquad y(x_0) = y_0, \qquad y'(x_0) = z_0, \tag{2.2}$$

for which an equivalent first order system is

$$
\begin{aligned}
y'(x) &= z(x), & y(x_0) &= y_0, \\
z'(x) &= f(y), & z(x_0) &= z_0.
\end{aligned}
$$

This can be solved by a standard Runge–Kutta method but the number of evaluations of the function f is lower if it is solved by a method specifically designed for (2.2).

3. The order of Runge–Kutta methods

In the famous papers of Runge [32] and Kutta [26], the idea of repeatedly substituting into the differential equation to obtain a sequence of approximate solutions was developed. Runge considered the scalar differential equation

$$y' = f(x, y),$$

and generalized this to the system

$$y' = f(x, y, z), \qquad z' = g(x, y, z).$$

He showed how to generalize the midpoint and trapezoidal quadrature rules into methods for these problems. Kutta systematically found the order conditions as far as order 5 and found methods of up to this order. Further work on Runge–Kutta methods was carried out by E.J. Nyström [30] and by A. Huťa [24] who took the analysis as far as order 6. For this order there are 31 order conditions for a single first order equation but 37 for a general system. The theory for a system, which we will now discuss, comes out of the work of S. Gill [19], of R.H. Merson [28] and of the present author [6].

Let T denote the set of all rooted trees, and let the "order" $r(t)$ denote the number of vertices for $t \in T$. For $r(t) > 1$, let $t_1, t_2, \ldots, t_m$ be the (rooted) trees formed by deleting the root, supposed to have degree m, from t. We denote the relationship between t and $t_1, t_2, \ldots, t_m$ by the notation $t = [t_1, t_2, \ldots, t_m]$. If τ is the unique tree with only a single vertex, then all trees can be expressed in terms of τ and the symbols [and]. For example, the eight trees of orders up to 4 can be written respectively as τ, $[\tau]$, $[\tau, \tau]$, $[[\tau]]$, $[\tau, \tau, \tau]$, $[\tau, [\tau]]$, $[[\tau, \tau]]$ and $[[[\tau]]]$. Define the "symmetry" of t by $\sigma(t) = m_1! m_2! \cdots m_k! \sigma(t_1)\sigma(t_2)\cdots\sigma(t_m)$, where m_1 of $t_1, t_2, \ldots, t_m$ are identical of one kind, m_2 are identical of a second kind, ..., and m_k are identical of a final kind. The recursive definition of σ is started with the value $\sigma(\tau) = 1$. The "density" of t is defined by $\gamma(t) = r(t)\gamma(t_1)\gamma(t_2)\cdots\gamma(t_m)$, with $\gamma(\tau) = 1$. For $t \in T$ and $v \in \mathbb{R}^N$ define the "elementary differential" associated with the function $f\colon \mathbb{R}^N \to \mathbb{R}^N$ and the tree t by

$$F(t)(u) = f^{(m)}(u)\left(F(t_1)(u), F(t_2)(u), \ldots, F(t_m)(u)\right),$$

with $F(\tau)(u) = f(u)$.

With this terminology, the formal Taylor series for the solution to the dimensional differential equation

$$y'(x) = f(y(x)),$$

with initial value

$$y(x_0) = y_0,$$

is given by

$$y(x_0 + h) = y(x_0) + \sum_{t \in T} h^{r(t)} \frac{1}{\sigma(t)\gamma(t)} F(t)(y_0). \tag{3.1}$$

For a given Runge–Kutta method, with array

$$\begin{array}{c|ccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

introduce the "elementary weights" associated with t. For stage number i this will be denoted by $\Phi_i(t)$ and, for the overall method, by $\Phi(t)$. These are defined by the recursions

$$\Phi_i(\tau) = \sum_{j=1}^{s} a_{ij} = c_i,$$

$$\Phi(\tau) = \sum_{j=1}^{s} b_j,$$

$$\Phi_i([t_1, t_2, \ldots, t_m]) = \sum_{j=1}^{s} a_{ij} \prod_{k=1}^{m} \Phi_j(t_k),$$

$$\Phi([t_1, t_2, \ldots, t_m]) = \sum_{j=1}^{s} b_j \prod_{k=1}^{m} \Phi_j(t_k).$$

The formal series for the computed solution at $x_0 + h$ is given by

$$y(x_0) + \sum_{t \in T} h^{r(t)} \frac{\Phi(t)}{\sigma(t)} F(t)(y_0). \tag{3.2}$$

Comparing the two series (3.1) and (3.2), we find the conditions for order p as

$$\Phi(t) = \frac{1}{\gamma(t)}, \tag{3.3}$$

which is to hold for all trees up to order p.

To prove formally that these sufficient conditions are also necessary, requires an analysis of the elementary differentials. It would need to be shown that they are independent, in the sense that, given a finite set of rooted trees, there exists a choice of the function f, such that some component can take on arbitrary values for members of the given set of trees. A proof of this is given in [9].

As we have remarked, for a single first order differential equation, the order conditions are less restrictive so that evidently the independence does not hold in this case. It is interesting to note that the order conditions up to $p = 4$ are identical for the general system and for the single first order (nonautonomous) equation. For order 5, there is one less condition for the single equation case (16 rather than 17 conditions) and for order 6, there are 6 less conditions for the single equation (31 rather than 37 conditions).

By taking a set of independent linear combinations of the order conditions, alternative formulations are possible. In recent work of Albrecht [1] such a formulation is developed. For example, instead of

$$\sum_{i,j=1}^{s} b_i a_{ij} c_j = \frac{1}{6}, \tag{3.4}$$

the condition

$$\sum_{i=1}^{s} b_i \left(\sum_{j=1}^{s} a_{ij} c_j - \frac{c_i^2}{2} \right) = 0, \tag{3.5}$$

must be satisfied. The conditions (3.4) and (3.5) are equivalent because the quadrature condition

$$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3},$$

must also hold. The derivation of conditions such as this is carried out in a completely different manner from that given here and the reader is referred to the work of Albrecht [1] or to the text-book by Lambert [27] for the details.

4. The search for high orders

High order methods are capable of achieving highly accurate approximations of differential equations solutions at lower computational cost than low order methods. For linear multistep methods of Adams–Bashforth and Adams–Moulton types, the construction of methods of any order is a routine matter. The fact that there is no automatic construction method for (explicit) Runge–Kutta methods of a given

Table 1

p	s	Author	Year		Reference
2	2	Runge	1895		[32]
3	3	Heun	1900		[23]
4	4	Kutta	1901		[26]
5	6	Kutta	1901		[26]
5	6	Nyström	1925	(correction to Kutta)	[30]
6	8	Huťa	1956		[24]
6	7	Butcher	1964		[7]
7	9	Butcher		(known since approximately 1968)	[9]
8	11	Curtis	1970		[12]
8	11	Cooper and Verner	1972	(announced 1969 in J.H. Verner's thesis)	[10]
10	18	Curtis	1975		[13]
10	17	Hairer	1978		[20]

order with a minimum number of stages makes the search for methods of higher and higher order an interesting challenge. For given order p it is not known in general how large the number of stages s must be to achieve this order.

For orders 1, 2, 3 and 4, the lowest possible number of stages is $s = p$. However, for $p = 5$ and $p = 6$, the lowest possibility is $s = p + 1$. For, $p = 7$, $s = 9$ stages are necessary whereas for $p = 8$, the minimum number of stages is $s = 11$. Above this, very little is known.

Table 1 shows some details of the chronology of attempts to obtain increasingly high orders.

5. Implicit Runge–Kutta methods

Implicit Runge–Kutta methods were proposed by Kuntzmann [25] and by Butcher [8] with the central example being methods based on Gaussian quadrature formulae. The remarkable thing about these methods is that the order, $p = 2s$, for an s stage method is exactly the same as for a pure quadrature problem. Also remarkable is that they are all A-stable. To construct such a method all that is required is to select the abscissae $c_1, c_2, \ldots, c_s$, as the zeros of the shifted Legendre polynomial on the interval $[0, 1]$ and to select each row of the A matrix and the vector b^T so that each of the quadrature formulae

$$\int_0^{c_i} \phi(x)\,dx \approx \sum_{j=1}^{s} a_{ij}\phi(c_j), \quad i = 1, 2, \ldots, s,$$

$$\int_0^{1} \phi(x)\,dx \approx \sum_{j=1}^{s} b_j\phi(c_j),$$

is exact for ϕ any polynomial of degree not exceeding $s-1$. The most famous example, which precedes the general introduction of the Gauss–Legendre methods [22], is given by

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

A variety of alternatives to these methods, based on the quadrature rules of Radau and of Lobatto, have also been introduced. These share with the Gauss–Legendre methods the advantages of high order and good stability. However, they also share the serious disadvantage of being extremely costly to implement for stiff problems.

Some alternatives to full implicitness have been suggested and strongly promoted. One of these proposals is the use of Rosenbrock methods, in which the Jacobian function formed from the function f plays an integral part in the computation, but where the method is otherwise explicit. However, these are not Runge–Kutta methods and, important as they are, they do not fit within the scope of this history.

What have been variously named "semi-implicit Runge–Kutta methods", "semi-explicit Runge–Kutta methods" [29], "diagonally-implicit Runge–Kutta methods" (DIRK) [2], and "singly-diagonally-

implicit Runge–Kutta methods" (SDIRK), also have a following. The idea here is to restrict the method to the form

$$\begin{array}{c|ccccc} c_1 & \lambda & 0 & 0 & \dots & 0 \\ c_2 & a_{21} & \lambda & 0 & \dots & 0 \\ c_3 & a_{31} & a_{32} & \lambda & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ c_s & a_{s1} & a_{s2} & a_{s3} & \dots & \lambda \\ \hline & b_1 & b_2 & b_3 & \dots & b_s \end{array}$$

so that the stages can be evaluated in sequence.

This idea leads to some highly efficient A-stable methods, but as the order increases, the methods become increasingly complicated. They also suffer from an "order-reduction" phenomenon.

Closely related methods are the singly-implicit methods, in which $\sigma(A)$ is constrained to be a set of eigenvalues with only a single member. Using a transformation technique, these methods are capable of achieving close to the efficient implementation properties of SDIRK methods without loss of stage-order.

The order-reduction phenomenon that has been referred to above has been studied by a number of authors starting from [31]. A recent survey of this work, including the theory of "B-convergence" first announced in [17], is the subject of [16].

6. Stability analysis

Because of the need to solve stiff problems using implicit Runge–Kutta methods, or for that matter mildly-stiff problems using explicit Runge–Kutta methods, stability regions play an essential part in the assessment of individual methods. For a method given by the tableau

$$\begin{array}{c|c} c & A \\ \hline & b \end{array},$$

the stability region for a linear problem $y' = qy$ is easily found. Write $z = hq$ and the vector of stage values satisfies

$$Y = y_0 e + zAY,$$

where $e = [1, 1, 1, \dots, 1]^{\mathrm{T}}$, leading to the value of y_1 computed in a single step as

$$y_1 = y_0 + zb^{\mathrm{T}}Y = y_0 + y_0 zb^{\mathrm{T}}(I - zA)^{-1}e = R(z)y_0.$$

The "stability function", $R(z)$, is given by the formula

$$R(z) = 1 + zb^{\mathrm{T}}(I - zA)^{-1}e.$$

For explicit methods this can be written in the form

$$R(z) = 1 + zb^{\mathrm{T}}e + z^2 b^{\mathrm{T}}c + z^3 b^{\mathrm{T}}Ac + \cdots + z^s b^{\mathrm{T}}A^{s-2}c.$$

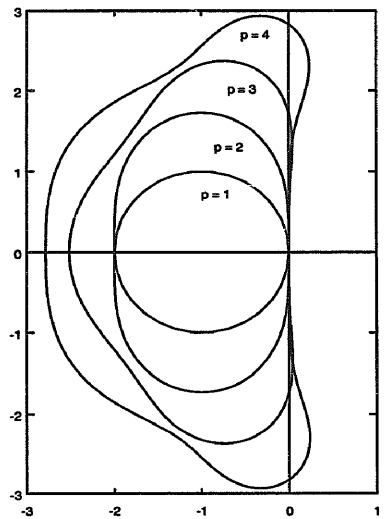

Fig. 1. Stability region boundaries for explicit Runge–Kutta methods.

If the order p equals the number of stages s, which we have seen is possible for $p \leqslant 4$, then $R(z)$ is precisely the truncated exponential series

$$R(z) = 1 + z + \frac{z^2}{2} + \frac{z^3}{3!} + \cdots + \frac{z^s}{s!},$$

and it is a simple matter to present the stability region as the set of points in the complex plane satisfying $|R(z)| \leqslant 1$. These are shown for $p = 1, 2, 3, 4$ in Fig. 1.

Because nonconstant polynomials are unbounded over unbounded subsets in the complex plane, stability regions are always bounded sets. This means that A-stability is impossible for explicit methods. For implicit Runge–Kutta methods, on the other hand, A-stability is achievable for the Gauss methods and for some closely related methods.

Suppose that the stability function R is a rational function with degrees r (numerator) and s (denominator) and suppose that the order is $p = r + s$. This implies that

$$R(z) - \exp(z) = O\left(z^{r+s+1}\right),$$

so that R is a Padé approximation to the exponential function. Methods possessing stability functions of this form are the Gauss methods (with $r = s$), the so-called Radau IA and IIA methods (in each case with $r = s$), and the Lobatto IIIC methods (with $r = s - 2$). Because of this relation, it is appropriate to study Padé approximations to the exponential function in their own right. An approximation is said to be "A-acceptable" if it is the stability function of an A-stable method. By the maximum modulus

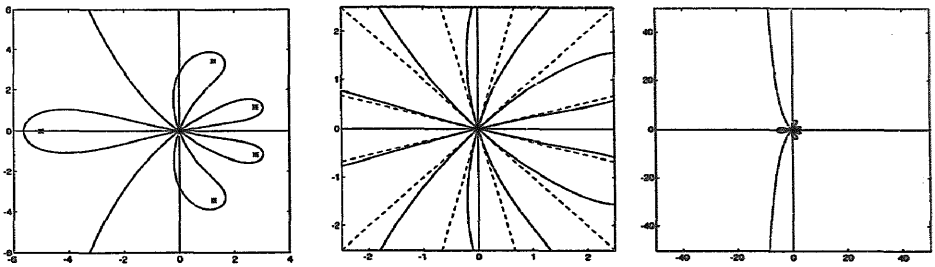

Fig. 2. Three views of contour lines for $R_{14}(z)\exp(-z)$.

principle, a rational approximation $R(z) = N(z)/D(z)$ is A-acceptable if and only if all zeros of D are in the right half-plane and if in addition $|D(iy)|^2 - |N(iy)|^2 \geqslant 0$ for all real y.

This property is now known to hold if and only if the degree of the numerator (say r) and the degree of the denominator (say s) satisfy the inequalities $0 \leqslant s - r \leqslant 2$. This was proved for the case $r = s$ by Birkhoff and Varga [3]. For a review of the other cases where A-acceptability occurs, see the book by Hairer and Wanner [21]. For the non-A-acceptable cases, those for which $r > s$ are a consequence of the limit $|R(z)| \to \infty$ as $|z| \to \infty$. The cases satisfying $s > r + 2$ can be proved using the technique of "order stars" [36]. Although it is not possible to discuss the details here, three figures are presented to motivate this approach (see Fig. 2). In each case the boundary of the "relative stability region" for the $(1,4)$ Padé approximation relative to the exponential function is shown. That is, the set of points in the complex plane is shown for which

$$\left|\frac{1 + z/5}{1 - 4z/5 + 3z^2/10 - z^3/15 + z^4/120}\exp(-z)\right| = 1.$$

In the left-hand view, four poles can be seen in the positive half-plane and one zero in the negative half-plane. It can be shown that the bounded "fingers" (the set of points for which $|R(z)| > |\exp(z)|$) each has a corresponding pole and the bounded "dual-fingers" (the set of points for which $|R(z)| < |\exp(z)|$) each has a corresponding zero. The fingers and dual-fingers originating from the origin in a method of order p subtend angles of $\pi/(p+1)$, as shown in the broken lines in the centre view. Finally, the distant view on the right indicates that for large values of z, the exponential factor dominates the shape of the boundary between relative stability and relative instability, so that for these large arguments the regions are divided approximately by the imaginary axis. The Padé approximation exemplified here, like other below the second subdiagonal are shown not to be A-stable because there must either be a pole in the left half-plane or else at least one of the bounded fingers must emerge from the origin at too great an angle from the positive real axis to lie completely in the right half-plane. However, such a finger must contain a pole in the right half-plane and hence must cross the imaginary axis, which is inconsistent with A-stability.

In the last 20 years, there has been some interest in requiring stricter stability properties than that yielded by the simple linear stability analysis that has been described here. Two separate generalizations

turn out to have similar consequences. The first of these is to allow for time-dependent linearity, so that the linear test model is

$$y'(x) = q(x)y(x),$$

where q is assumed to take only values in the left half-plane. The second generalization is to consider (possibly nonlinear) dissipative differential equations in an inner-product space. That is, assume the equation system is

$$y'(x) = f\big(x, y(x)\big),$$

where, for all x and all vectors u and v,

$$\big\langle f(x,u) - f(x,v), u - v\big\rangle \leqslant 0. \tag{6.1}$$

A sufficient condition for stable behaviour with either of these test problems is that each of b_1, b_2, $\ldots$, b_s is positive and that the $s \times s$ matrix M with (i,j) element equal to $b_i a_{ij} + b_j a_{ji} - b_i b_j$ is positive semidefinite. Under not particularly stringent restrictions, these conditions are also necessary [5,11].

The condition that M be positive semidefinite is known as "algebraic stability" whereas stable behaviour for (6.1) is known as "BN-stability" (or, if the differential equation is autonomous, as "B-stability").

Recent research on systems of differential equations arising from Hamiltonian dynamics, has given a new significance to M in that M must be the zero matrix if symplectic properties of the Hamiltonian system are to be inherited by a Runge–Kutta method used for its numerical approximation. The review paper [33] and the book [34] are recommended as references for this body of work.

7. Error estimates and continuous output

The combining of two methods, of different orders, into a single tableau was first proposed by Merson [28]. His idea was to construct a method with five stages for which a fourth order method could be found from the first four and a fifth order method from all the five stages. The difference of the two results so obtained would then be an asymptotically correct approximation to the local truncation error committed by the fourth order method. Unfortunately, it is not possible to obtain the two methods he sought within a total of 5 stages and he had to be content with a scheme in which the estimate of the local truncation error he obtained was only appropriate for problems which are approximately linear. In spite of this, the Merson method has had a loyal following as the basis of practical software for many years.

Within the last 30 years, many contributions have been made to the development of embedded pairs, as they are now named, for which the error estimate is asymptotically correct, but at the expense of additional stages compared with the Merson method. Notable is the early work of Fehlberg [15] who took the search for Runge–Kutta pairs as high as order 7. Other major contributors to this investigation include Verner [35] and Dormand and Prince [14].

The wish to obtain output at points internal to a step, without interrupting the natural flow of the computation, has led to methods which are embedded in a different way. In addition to the final result given by the tableau

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \vdots & & \vdots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array},$$

a further vector is added for which the elements depend on a parameter ξ. Denote the elements by

$$[\hat{b}_1(\xi)\ \hat{b}_2(\xi)\ \dots\ \hat{b}_s(\xi)],$$

and suppose that the method with the last row replaced by this vector is required to give an approximation to $y(x_0+\xi h)$. If the order of this internal approximation is $\hat{p}$, then the corresponding elementary weights, with b replaced by $\hat{b}(\xi)$ satisfy the equations

$$\widehat{\Phi}(t) = \frac{\xi^{r(t)}}{\gamma(t)},$$

for every tree t such that $r(t) \leqslant \hat{p}$.

Although many people have worked on the derivation of methods with this property, the first seems to have been Gear [18].

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